

4-Imidazolidinone, 5-methyl-2-thio-

Other names:	Hydantoin, 5-methyl-2-thio- 5-Methyl-2-thiohydantoin 5-Methyl-2-thioguidanthion
Inchi:	InChI=1S/C4H6N2OS/c1-2-3(7)6-4(8)5-2/h2H,1H3,(H2,5,6,7,8)
InchiKey:	HYDZMARBTYAIMU-UHFFFAOYSA-N
Formula:	C4H6N2OS
SMILES:	CC1N=C(S)N=C1O
Mol. weight [g/mol]:	130.17
CAS:	33368-94-4

Physical Properties

Property code	Value	Unit	Source
gf	186.14	kJ/mol	Joback Method
hf	55.40	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	62.50	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.631		Crippen Method
mcvol	89.940	ml/mol	McGowan Method
pc	6696.65	kPa	Joback Method
tb	576.92	K	Joback Method
tc	817.57	K	Joback Method
tf	412.66	K	Joback Method
vc	0.344	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.94	J/mol×K	576.92	Joback Method
cpg	230.34	J/mol×K	617.03	Joback Method
cpg	240.11	J/mol×K	657.14	Joback Method
cpg	249.21	J/mol×K	697.25	Joback Method
cpg	257.61	J/mol×K	737.35	Joback Method
cpg	265.30	J/mol×K	777.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33368944&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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